Chirally rotated Schrödinger functional: non-perturbative tuning in the quenched approximation

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The use of chirally rotated boundary conditions provides a formulation of the Schrödinger functional that is compatible with automatic $O(a)$ improvement of Wilson fermions in the bulk. The elimination of bulk $O(a)$ terms requires the non-perturbative tuning of the critical mass and one additional boundary counterterm. We present the results of such a tuning in the quenched approximation at three values of the renormalised gauge coupling and for a range of lattice spacings.

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1. Introduction

Obtaining precise physical results from lattice calculations requires a well controlled continuum limit and, for many quantities, non-perturbative renormalisation. Ideally the renormalisation scheme should be not only *non-perturbative* but also *mass independent* and preferably *gauge invariant*. Schrödinger functional (SF) schemes [1, 2, 3] are known to fulfill these properties. Additionally, to ease the burden of taking the continuum limit, $O(a)$ improvement is highly desirable. However, to eliminate the many counterterms necessary when applying the standard $O(a)$ improvement program with Wilson fermions, we would like to capitalize on the automatic $O(a)$ improvement provided by maximally twisted mass fermions [4] (see [5] for a review). Unfortunately, bulk automatic $O(a)$ improvement with Wilson fermions and the standard SF (sSF) boundary conditions (BCs) are not compatible. $O(a)$ improvement is only possible introducing a number of additional bulk improvement counter-terms to the action and operators. Since there are extensive calculations with maximally twisted mass fermions [6, 7] it would be clearly desirable to employ the SF scheme while keeping automatic $O(a)$-improvement.

A new formulation of the SF has been developed in Ref. [8], which we will refer to as the *c*hirally rotated SF (χSF), that implements a SF scheme while maintaining automatic $O(a)$ improvement for massless Wilson fermions. The χSF is related (in the continuum) to the sSF by means of a non-singlet chiral transformation, i.e. they are equivalent in the continuum limit. However, when using massless Wilson fermions as a lattice regulator, χSF BCs are invariant under a subgroup of the chiral symmetry transformations broken by the Wilson term (in contrast to sSF BCs). As a result χSF BCs are compatible with automatic $O(a)$ improvement.

The three-dimensional boundaries of the SF lead to an unavoidable dimension four boundary operator. Additionally, regulating the χSF with Wilson fermions induces the usual bulk mass operator as well as a dimension three boundary operator. The dimension four boundary operator is irrelevant, and hence the corresponding coefficient can be safely fixed by perturbation theory in order to eliminate the corresponding $O(a)$ boundary contributions. The bulk operator is relevant and is handled by the standard non-perturbative tuning of the bare quark mass, equivalently κ, to its critical value. The dimension three operator is also relevant and can spoil not only the automatic $O(a)$ improvement but also the universality of the continuum limit. This requires an additional non-perturbative tuning of one more counterterm, z_{f}. However, having tuned both κ and z_{f}, all operators are automatically $O(a)$ improved and no further counterterms are necessary.

Here we present the non-perturbative tuning of κ and z_{f} for the χSF in the quenched approximation. We demonstrate the feasibility of tuning both parameters simultaneously. In particular, the inclusion of the bulk dimension five operator, with corresponding counterterm c_{sw}, as used in Ref. [9], is found to be unnecessary.

2. Boundary conditions

The χSF is related to the sSF by a non-singlet chiral transformation, $\chi = \exp(-i\pi\gamma_5\tau^3/4)\psi$, where ψ is the fermion doublet in the $N_{\mathrm{f}} = 2$ standard formulation, χ is the corresponding doublet in the rotated basis and τ^3 is a Pauli matrix. This field transformation maps the sSF BCs to the χSF

BCs,

$$Q_+ \chi(x)|_{x_0=0} = 0 \qquad\qquad Q_- \chi(x)|_{x_0=T} = 0 \tag{2.1}$$

$$\overline{\chi}(x) Q_+|_{x_0=0} = 0 \qquad\qquad \overline{\chi}(x) Q_-|_{x_0=T} = 0,$$

where T is the Euclidean time extent and $Q_\pm$ are projectors given by

$$Q_\pm = \frac{1}{2}\left(\mathbb{1} \pm i\gamma_0\gamma_5\tau^3\right).$$

Thus the $Q_\pm$ are simply the chirally rotated projectors corresponding to the sSF projectors, $P_\pm = 1/2(1 \pm \gamma_0)$. However, once the theory is regularised on the lattice, we must ensure that the BCs in (2.1) are in fact recovered in the continuum limit. Using orbifolding techniques, it was shown that the BCs can be implemented at finite lattice spacing by a simple modification of the standard Wilson-Dirac operator, D_W, near the time boundaries [10]. The resulting action is

$$S = a^4 \sum_{x_0=0}^{T} \sum_{\tilde{x}} \overline{\chi}(x) \left(\mathscr{D}_W + m_0\right) \chi(x) \tag{2.2}$$

and the modified Wilson-Dirac operator is given by

$$a\mathscr{D}_W \chi(x) = \begin{cases} -U(x,0)P_-\chi(x+a\hat{0}) + (aK + i\gamma_5\tau^3 P_-)\chi(x) & \text{if} \quad x_0 = 0 \\ aD_W\chi(x) & \text{if} \quad 0 < x_0 < T \\ (aK + i\gamma_5\tau^3 P_+)\chi(x) - U^\dagger(x-a\hat{0},0)P_+\chi(x-a\hat{0}) & \text{if} \quad x_0 = T \end{cases} \tag{2.3}$$

where K is the time-diagonal contribution to D_W.

3. Boundary counterterms

To ensure the correct continuum limit, we must account for all relevant operators allowed by the symmetries of the action above. This means dimension four or less for the bulk action. There is one such operator, $\overline{\chi}\chi$, and the corresponding counterterm is the term proportional to the critical quark mass, m_{cr}, or equivalently κ_{cr}. This is the standard operator that is present for all Wilson actions due to the breaking of chiral symmetry by the Wilson term.

Similarly, we must include all permitted boundary operators of dimension three or less. Again, the one allowed operator is $\overline{\chi}\chi$ [8], which gives rise to the following counterterm to the lattice action,

$$\delta S_3 = (z_f - 1)a^3 \sum_{\vec{x}} \left(\overline{\chi}\chi|_{x_0=0} + \overline{\chi}\chi|_{x_0=T}\right).$$

Such an operator would be forbidden in the continuum action, but the reduced symmetries of the Wilson action do not allow us to exclude this operator on the lattice. The presence of δS_3 can then be understood as necessary to restore the symmetries broken by the Wilson term in the continuum limit. The fact that it is a relevant operator implies that we must compute the bare coupling dependence of z_f non-perturbatively, just as for κ.

Furthermore, we must examine those irrelevant operators that lead to $O(a)$ contributions. In the bulk, there is the dimension five Sheikholeslami-Wohlert term, but automatic $O(a)$ improvement eliminates the need for this operator. Yet, there does remain an $O(a)$ contribution from the boundary due to the irrelevant dimension four operator [9],

$$\delta S_4 = (d_{\mathrm{s}} - 1)a^4 \sum_{\vec{x}} \left(\overline{\chi}\gamma_k D_k \chi|_{x_0=0} + \overline{\chi}\gamma_k D_k \chi|_{x_0=T} \right).$$

Such a contribution is present in all SF formulations [3] and is not due to the particular lattice action or BCs we have chosen. In fact, d_{s} plays a role that is analogous to the $\tilde{c}_t$ counterterm in the sSF [11]. Given that δS_4 is an irrelevant operator, d_s can be computed in perturbation theory. For the investigation presented here, we simply use the tree-level value of $1/2$.

4. Tuning conditions

The non-perturbative determination of κ and z_{f} requires imposing conditions at finite lattice spacing that ensure the restoration of all expected symmetries in the continuum limit: parity and flavour symmetries in the $\chi-$ basis[1]. Moreover, these conditions should be imposed at each lattice spacing while fixing a suitable renormalised quantity. In this work, we keep the renormalised SF coupling, $\overline{g}$, fixed. This is equivalent to fixing the physical size of the box, L. All other dimensionful quantities must scale with L, so we choose $T = L$, evaluate all correlation functions at $x_0 = T/2$ and use periodic boundary conditions with $\theta = 0$.

Before specifying the tuning conditions, we define the following boundary to bulk correlation functions

$$g_{\mathrm{A}_\pm}^{ab}(x_0) = -\langle A_0^a(x)\mathcal{Q}_\pm^b \rangle \qquad g_{\mathrm{P}_\pm}^{ab}(x_0) = -\langle P^a(x)\mathcal{Q}_\pm^b \rangle$$

where the boundary operator, $\mathcal{Q}_\pm^a$, is defined for the $x_0 = 0$ boundary by

$$\mathcal{Q}_\pm^a = a^6 \sum_{\vec{y},\vec{z}} \overline{\zeta}(\vec{y})\gamma_5 \frac{1}{2}\tau^a Q_\pm \zeta(\vec{z}) e^{i\vec{p}(\vec{y}-\vec{z})},$$

the bulk operators $A_\mu^a(x)$ and $P^a(x)$ are the axial current and pseudoscalar density in the χ-basis, and the boundary fields for $x_0 = 0$ are defined as

$$\zeta(\vec{x}) = U(x_0-a,\vec{x};0)\chi(x)|_{x_0=a} \qquad \overline{\zeta}(\vec{x}) = \overline{\chi}(x)U^\dagger(x_0-a,\vec{x};0)|_{x_0=a}.$$

To tune κ to its critical value, we adopt the standard procedure of imposing a vanishing PCAC mass. To tune z_{f}, we require the $\gamma_5\tau_1$-odd correlation function $g_{\mathrm{A}_-}^{11}$ to vanish,

$$m_{\mathrm{PCAC}} \equiv \frac{\partial_0^{\mathrm{latt}} g_{\mathrm{A}_-}^{11}(T/2)}{2g_{\mathrm{P}_-}^{11}(T/2)} = 0 \qquad g_{\mathrm{A}-} \equiv g_{\mathrm{A}_-}^{11}(T/2) = 0. \tag{4.1}$$

The second condition in particular is sensitive to the symmetries broken by the lattice action (2.2), and both conditions together ensure that in the continuum limit all broken symmetries are indeed restored. Imposing different symmetry restoration conditions would give rise to different values of κ and z_{f} that would differ amongst themselves by cutoff effects. It will be important to study the sensitivity of κ and z_{f} to the particular definitions used in order to better understand the intrinsic uncertainty in the determination of these counterterms.

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[1]We recall that in the $\chi-$ basis parity and flavour symmetries take a slightly different form (see ref. [5] for a discussion about the dependence of the symmetries on the basis adopted).

L/a	β	z_{f}^{*} (χSF)	κ_{cr} (χSF)	κ_{cr} (sSF)
Tuning at a hadronic scale, $\mu \sim 300$ MeV
8	6.0219	1.8090 (32)	0.153530 (24)	0.153371 (10)
10	6.1628	1.7920 (30)	0.152134 (17)	0.152012 (7)
12	6.2885	1.7664 (51)	0.150815 (22)	0.150752 (10)
16	6.4956	1.7212 (83)	0.148945 (25)	0.148876 (13)
Tuning at an intermediate scale, $\mu \sim 1$ GeV
8	7.0197	1.5467 (15)	0.144501 (13)	0.144454 (7)
12	7.3551	1.5126 (23)	0.143113 (12)	0.143113 (6)
16	7.6101	1.4942 (37)	0.142112 (13)	0.142107 (6)
Tuning at a perturbative scale, $\mu \sim 30$ GeV
8	10.3000	1.29730 (67)	0.1354609 (54)	0.135457 (5)
12	10.6086	1.2954 (11)	0.1351758 (56)	0.135160 (4)
16	10.8910	1.2858 (15)	0.1348440 (61)	0.134849 (6)

Table 1: Tuning results at a hadronic, intermediate and perturbative scale. We give the critical values, z_{f}^{*} and κ_{cr}, calculated in this work for the χSF. For reference, we also give κ_{cr} for the sSF [12, 13, 14].

5. Tuning results

To check the practicality of tuning both κ and z_{f} non-perturbatively for the χSF, we perform the tuning at three values of the renormalisation scale $\mu = 1/L$, corresponding to a hadronic ($\overline{g}^2$ fixed with $L = 1.436 r_0$), an intermediate ($\overline{g}^2 = 2.4484$) and a perturbative ($\overline{g}^2 = 0.9944$) scale. The results at these three points are summarised in Tab. 1. We now briefly explain the procedure we used to perform the tuning, showing examples from our most difficult point at the hadronic scale and for the smallest lattice, $L/a = 8$.

The values of β used are given in Tab. 1 and are taken from Ref. [15]. The tuning is performed in several steps. First, we calculate m_{PCAC} and $g_{\mathrm{A}-}$ at four values of z_{f}, and for each value of z_{f}, we use four values of κ, thus giving 16 pairs of κ and z_{f}. This allows us to determine $g_{\mathrm{A}-}$ as a function of m_{PCAC} for each value of z_{f}, as illustrated in Fig. 1. For each value of z_{f}, we perform a linear interpolation of $g_{\mathrm{A}-}$ in terms of m_{PCAC} to the point $m_{\mathrm{PCAC}} = 0$. This determines the values of $g_{\mathrm{A}-}$ at $m_{\mathrm{PCAC}} = 0$ for each of the four values of z_{f}, as shown in Fig. 2. We now interpolate these values of $g_{\mathrm{A}-}$ as a function of z_{f} to the point of vanishing $g_{\mathrm{A}-}$, thus giving us the critical value z_{f}^{*}.

Next we determine κ_{cr}. Using the same 16 pairs of κ and z_{f}, we calculate m_{PCAC} as a function of κ for each z_{f}. This is shown in Fig. 3. Note that m_{PCAC} has a very mild dependence on z_{f}, so the four curves at fixed z_{f} are nearly indistinguishable. Interpolating in κ to the point of vanishing PCAC mass, we obtain the critical values of κ at each z_{f}. The resulting values of κ as a function of z_{f} are shown in Fig. 4. We now interpolate these results in z_{f} to the previously determined value of z_{f}^{*}, thus determining the value of κ_{cr}.

A key observation of this work is the mild dependence of m_{PCAC} on z_{f}, at least in the region near κ_{cr} and z_{f}^{*}. You can easily see this in Fig. 3. The consequence of this is clear in Fig. 4: the determination of κ_{cr} also has a weak dependence on z_{f}^{*} and the errors of both are relatively
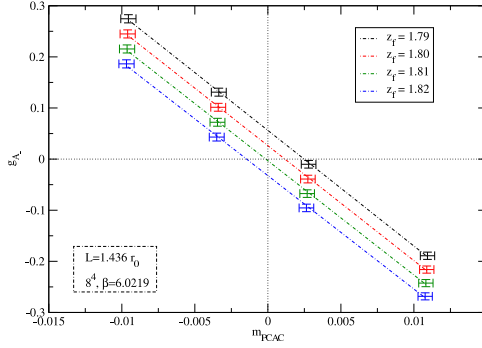
Figure 1: Plot of g_{A-} versus m_{PCAC}.
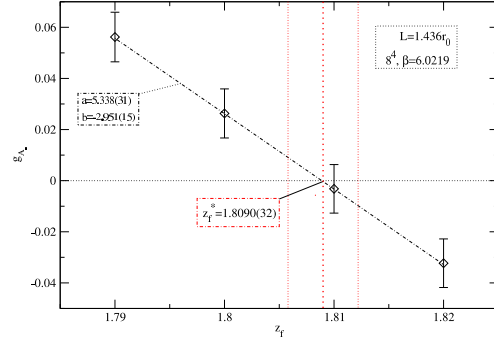
Figure 2: Plot of g_{A-} versus z_f.
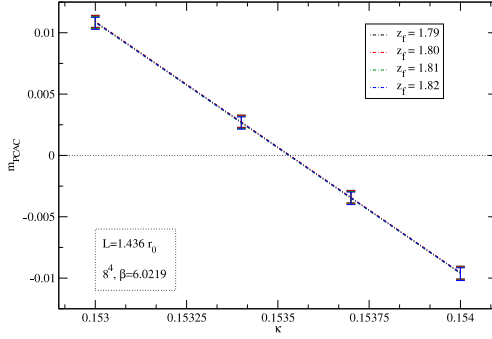
Figure 3: Plot of m_{PCAC} versus κ.
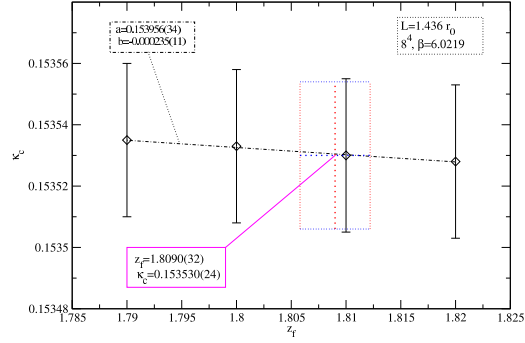
Figure 4: Plot of κ_{cr} versus z_f.

independent. If this behaviour persists with dynamical calculations, it could ease the numerical effort necessary to perform the tuning, thus reducing the number of required simulations.

6. Conclusions

We have presented the results of the non-perturbative tuning of κ and z_f for the χSF at three physical scales and for a range of lattice spacings. This demonstrates that the tuning of these two coefficients is indeed feasible, at least in the quenched approximation. Moreover, we observe that the tuning of z_f and κ are nearly independent. Note that even with non-improved Wilson fermions in the bulk, κ and z_f are the only parameters that must be tuned within the χSF setup in order to guarantee bulk automatic $O(a)$ improvement, thus eliminating the need for the bulk counterterm, c_{sw}, and for the many operator improvement coefficients necessary in the sSF.

Our next step is to perform an universality test of this formulation as well as a demonstration that automatic $O(a)$ improvement holds. This can be done by reproducing a variety of quantities already computed in the standard setup. A natural candidate would be the computation of the step-scaling function of the pseudoscalar renormalisation factor, Z_P, which could be compared to the

results of [15]. We recall that the χSF and the sSF are equivalent in the continuum limit, therefore, it is not necessary to recompute the entire evolution of an operator. The only quantity that must be recomputed is the renormalisation factor at the most non-perturbative scale.

We also plan to explore whether the value of κ_{cr} determined from the finite volume simulations can be used in large volume, preserving the nice scaling behaviour obtained in Refs. [16, 17], without the need for a large volume determination of κ_{cr}. A lattice perturbation theory computation of d_s and z_f is also planned. The final goal is to perform dynamical simulations.

Acknowledgments

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